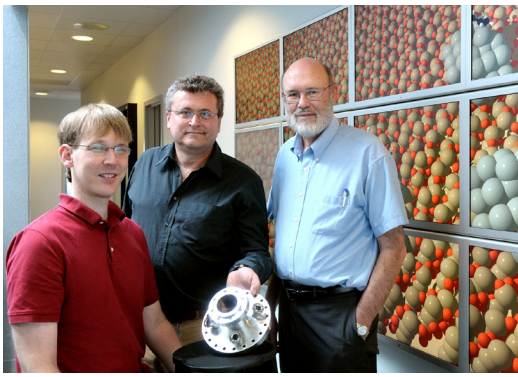
Scientists Develop Green Method to Produce Propylene Oxide

Propylene oxide is commonly used in the manufacturing of plastics and propylene glycols for paints, household detergents and automotive brake fluids.

The Challenge

The current production of propylene oxide creates a significant amount of by-products that are harmful to the environment, including chlorinated or peroxycarboxylic waste, or use expensive reagents, such as hydrogen peroxide.

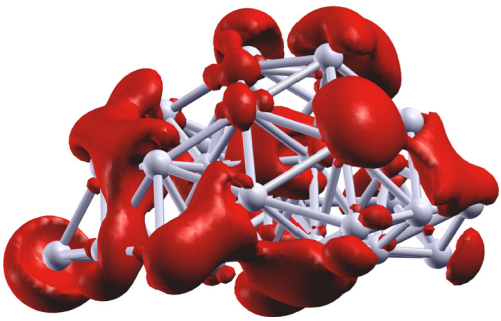
Manufacturers have tried using large silver particles to produce propylene oxide from propylene, but this method suffers from a low selectivity or low conversion to propylene oxide—creating a large amount of carbon dioxide.



Argonne scientists (from left) Jeff Greeley, Stefan Vajda and Larry Curtiss have developed a new way of creating propylene oxide that eliminates the many environmentally unfriendly by-products.

The Solution

Argonne researchers discovered that nanoscale clusters of silver, consisting of both three-atom clusters as well as larger nanostructures of 3.5 nanometers in size made of three-atom clusters, are highly active and selective catalysts for the production of propylene oxide. They then modeled the underlying mechanism behind why these ultrasmall nanoparticles of silver were so effective in creating propylene oxide. The researchers discovered that the open shell electronic structure of the silver catalysts was the impetus behind the nanoclusters' selectivity.



Calculated relaxed structure and spin densities of a Ag_{33} cluster. The optimized "nanohill" geometries are very disordered and suggest that the 2x4nm agglomerated nanoparticles might have core-shell structures. The high-spin states show significant spin density on some surface atoms, which are expected to be more active for propylene epoxidation as on the silver trimers.

The Results

Argonne scientists identified a new means of producing propylene oxide that is both more environmentally friendly and less expensive than current production methods. The new class of silver-based catalysts can produce the chemical with few by-products at low temperatures.

The findings resulted from a highly collaborative team that involved five Argonne divisions and collaborators from the Fritz-Haber-Institut in Berlin and the University of Illinois at Chicago.

"Propylene oxide is a building block in the creation of several other industrially relevant chemicals, but the current methods of creating it are not efficient," **said Larry Curtiss, Argonne materials chemist.** ***"The work opens a new chapter in the field of silver as a catalyst for propene epoxidation."***

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